Exact solutions of the radial Schrödinger equation for some physical potentials

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Abstract

By using an ansatz for the eigenfunction, we have obtained the exact analytical solutions of the radial Schrödinger equation for the pseudoharmonic and Kratzer potentials in two dimensions. The energy levels of all the bound states are easily calculated from this eigenfunction ansatz. The normalized wavefunctions are also obtained.

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1 Introduction

It is well known that the study of exactly solvable problems has attracted much attention since the early study of non-relativistic quantum mechanics. The exact solutions of the Schrödinger equation for a hydrogen atom (Coulombic) and for a harmonic oscillator in three dimensions as well as in an arbitrary number of spatial D-dimensions represent two typical examples in quantum mechanics [1-4]. The pseudoharmonic and Mie-type potentials [5,6] are also two exactly solvable potentials other than the Coulombic and anharmonic oscillator. In general, there are

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a few main methods to study the exact solutions of quantum mechanical systems. The first traditional method is to solve the second order differential Schrödinger equation by transforming it into some well known ordinary differential equations, whose solutions are the special functions like the confluent hypergeometric functions, associated Laguerre polynomials, the Whittaker functions and others [2]. The second method is related with the SUSYQM method, further closely with the factorization method [7]. The exact quantization rule also shown its power in calculating the energy levels of all the bound states for some exactly solvable quantum systems such as, the Morse, the Rosen-Morse, the Kratzer, the harmonic oscillator, the first and second Pöschl-Teller and the pseudoharmonic oscillator potentials [8-10]. The Nikiforov-Uvarov method [11] which is introduced for the solution of Schrödinger equation, to its energy levels, by transforming it into hypergeometric type second order differential equations. The method is based on the determination of the solution of wavefunction in terms of special orthogonal functions for any general second-order differential equation [12-15]. Also, the perturbative method introduced for calculating the energy levels of some bound states of the Schrödinger equation for some approximately solvable quantum systems [16-19]. Further, the exact solution of the D-dimensional Schrödinger equation with some anharmonic, pseudoharmonic and Kratzer potentials are obtained by applying an ansatz to the wavefunction [20,21].

Özçelik and Şimşek have proposed an ansatz for eigenfunction and presented the exact analytical solution of radial Schrödinger equation in three-dimensions of all the bound states with inverse-power potentials [22]. Moreover, by applying this factorization ansatz to the eigenfunction, Dong has carried out an exact analytical solutions of the Schrödinger equation in two-dimensions for some physical inverse-power potentials [23].

It is well known in quantum mechanics, a total wave function provides implicitly all relevant information about the behaviour of a physical system. Hence if it is exactly solvable for a given potential, the wave function can describe such a system completely. Until now, many efforts have been made to solve the stationary Schrödinger equation with anharmonic potentials in three dimensions and two dimensions. With the same spirit, in this work, we apply the method to study the solutions of the Schrödinger equation in two-dimensions for some pseudoharmonic and the modified Kratzer potentials due to their applications in physics [5,6,8,10,21,24].

This paper is organized as follows. In Section 2, we apply the factorization ansatz to the eigenfunction to obtain an exact analytic solution to the stationary radial Schrödinger equation in two-dimensions for the molecular pseudoharmonic

and modified Kratzer-Fues potentials. We also obtain the bound state eigensolutions of these molecular diatomic potentials by making a suitable ansatz to every wave function. The concluding remarks will be given in Section 3.

2 Wavefunction Ansatz

Consider the two-dimensional stationary Schrödinger equation with a potential $V(\rho)$ depending only on the distance ρ from the origin [25]:

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(\rho)\right)\psi(\rho,\varphi) = E\psi(\rho,\varphi), \tag{1}$$

leads to the following equation for the radial part of the wave function [25,26]:

$$\left[\frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\varphi^2} + \frac{2\mu}{\hbar^2}\left(E - V(\rho)\right)\right]\psi(\rho,\varphi) = 0. \tag{2}$$

On expressing the wave function as the product

$$\psi(\rho,\varphi) = r^{-1/2}R_m(\rho)\exp(\pm im\varphi),\ m = 0,1,2,\cdots, \tag{3}$$

the resulting differential equation for $R_m(\rho)$ reads

$$\left[\frac{d^2}{d\rho^2} + \frac{2\mu}{\hbar^2}\left(E - V(\rho)\right) - \frac{(m^2 - 1/4)}{\rho^2}\right]R_m(\rho) = 0, \tag{4}$$

where m and E denotes the angular momentum and the energy spectra, respectively. From the works [22,23], the radial wavefunction $R_m(\rho)$ has the following ansatz:

$$R_m(\rho) = f_m(\rho)\exp\left[g(\rho)\right], \tag{5}$$

where

$$f_m(\rho) = \begin{cases} 1 & \text{when } m = 0, \\ \prod_{j=1}^{m}(\rho - \alpha_j^{(m)}) & \text{when } m = 1,2,3,\cdots \end{cases} \tag{6}$$

and

$$g(\rho) = a\rho^2 + b\ln\rho,\ a < 0. \tag{7}$$

On inserting Eq.(5) into Eq.(4), one obtains

$$R_m''(\rho) - \left[g''(\rho) + (g'(\rho))^2 + \left(\frac{f_m''(\rho) + 2f_m'(\rho)g'(\rho)}{f_m(\rho)} \right) \right] R_m(\rho) = 0, \qquad (8)$$

where the prime denotes the derivative with respect to the variable ρ. Following the Refs [27,28] it is found from Eq. (4) that $R_m''(\rho)$ can be expressed as

$$-\frac{2\mu}{\hbar^2}E + \frac{2\mu}{\hbar^2}V(\rho) + \frac{(m^2 - 1/4)}{\rho^2} = g''(\rho) + (g'(\rho))^2 + \frac{f_m''(\rho) + 2f_m'(\rho)g'(\rho)}{f_m(\rho)}, \quad (9)$$

which is the most fundamental equation for the following analysis.

2.1 The pseudoharmonic potential

This potential has been studied in three dimensions [5] using the polynomial solution method and in D-dimensions using an ansatz for the wave function [21]. It has the following form [5,21]:

$$V(\rho) = D_e \left(\frac{\rho}{\rho_e} - \frac{\rho_e}{\rho} \right)^2, \qquad (10)$$

which can be simply rewritten in the form of isotropic harmonic oscillator plus inverse quadratic potential [5,10,29] as

$$V(r) = A\rho^2 + \frac{B}{\rho^2} + C, \; A, B > 0, \qquad (11)$$

where $A = D_e \rho_e^{-2}$, $B = D_e \rho_e^2$ and $C = -2D_e$.

First of all, we study the ground state ($m = 0$) so that we take $f_0(\rho) = 1$ and $g(\rho)$ in Eq. (7) to solve Eq. (9)

$$C' - E' + A'\rho^2 + \frac{B' + m^2 - \frac{1}{4}}{\rho^2} = 2a\,(1 + 2b) + 4a^2\rho^2 + \frac{b\,(b-1)}{\rho^2}, \qquad (12)$$

where $E' = \frac{2\mu}{\hbar^2}E$, $A' = \frac{2\mu}{\hbar^2}A$, $B' = \frac{2\mu}{\hbar^2}B$ and $C' = \frac{2\mu}{\hbar^2}C$. On equating coefficients of ρ^p, in Eq. (12), for all $p = -2, 0, 2$, the relations between the potential parameters and the coefficients a and b are as follows:

$$B' - \frac{1}{4} = b^2 - b, \; A' = 4a^2, \; -E' + C' = 2a(1 + 2b). \qquad (13)$$

Hence, we find from the first equation in (13) that $b = \frac{1}{2} + \sqrt{B'}$ and from the second equation, $a = \pm\frac{\sqrt{A'}}{2}$, but only the negative root yields a regular wave function at $\rho = 0$, and of course we choose $a = -\frac{\sqrt{A'}}{2}$ so that $A' > 0$. Finally, from the third equation in (13), the energy is

$$E_0 = C + \sqrt{\frac{2\hbar^2 A}{\mu}}\left(1 + \sqrt{\frac{2\mu B}{\hbar^2}}\right), \tag{14}$$

and the corresponding eigenfunction, by virtue of Eq. (3), can be written as

$$\psi_0(\rho,\varphi) = N_0 \exp\left[-\frac{1}{2}\sqrt{\frac{2\mu A}{\hbar^2}}\rho^2\right]\rho^{\sqrt{\frac{2\mu B}{\hbar^2}}}. \tag{15}$$

Secondly, for the first node $(m = 1)$, we use $f_1(\rho) = \rho - \alpha_1^{(1)}$ and $g(\rho)$ given in Eq. (7) to solve Eq. (9),

$$C' - E' + A'\rho^2 + \frac{B' + \frac{3}{4}}{\rho^2} = 2a\,(3 + 2b) + 4a^2\rho^2 + \frac{b\,(b+1)}{\rho^2}. \tag{16}$$

The relations between the potential parameters and the coefficients a, b and $\alpha_1^{(1)}$ are

$$B' + \frac{3}{4} = b^2 + b,\ A' = 4a^2, -E' + C' = 2a(3 + 2b),\ \alpha_1^{(1)} = 0, \tag{17}$$

which are solved as

$$b = -\frac{1}{2} + \sqrt{B' + 1}, a = -\frac{1}{2}\sqrt{A'},\ E_1' = C' + \sqrt{A'}(3 + 2b). \tag{18}$$

So that the energy eigenvalue reads

$$E_1 = C + \sqrt{\frac{2\hbar^2 A}{\mu}}\left(1 + \sqrt{\frac{2\mu B}{\hbar^2} + 1}\right), \tag{19}$$

and the corresponding eigenfunction can be written as (cf. (3))

$$\psi_1(\rho,\varphi) = N_1 \exp\left[-\frac{1}{2}\sqrt{\frac{2\mu A}{\hbar^2}}\rho^2\right]\rho^{\sqrt{\frac{2\mu B}{\hbar^2}+1}}e^{\pm i\varphi}. \tag{20}$$

We follow the same steps for the second node ($m = 2$) (i.e. $f_2(\rho) = (\rho - \alpha_1^{(2)})(\rho - \alpha_2^{(2)})$) and $g(\rho)$ is defined in Eq.(7) which imply that the following algebraic equation holds

$$C' - E' + A'\rho^2 + \frac{B' + \frac{15}{4}}{\rho^2} = 2a\left(5 + 2b\right) + 4a^2\rho^2 + \frac{\left(b+1\right)\left(b+2\right)}{\rho^2}, \tag{21}$$

which leads to equations

$$B' + \frac{15}{4} = \left(b+1\right)\left(b+2\right),\ A' = 4a^2,\ -E' + C' = 2a(5+2b), \alpha_1^{(2)} = \alpha_2^{(2)} = 0. \tag{22}$$

Therefore, the energy eigenvalue is

$$E_2 = C + \sqrt{\frac{2\hbar^2 A}{\mu}}\left(1 + \sqrt{\frac{2\mu B}{\hbar^2} + 4}\right), \tag{23}$$

and the eigenfunction reads

$$\psi_2(\rho, \varphi) = N_2 \exp\left[-\frac{1}{2}\sqrt{\frac{2\mu A}{\hbar^2}}\rho^2\right] \rho^{\sqrt{\frac{2\mu B}{\hbar^2}+4}} e^{\pm i2\varphi}. \tag{24}$$

It is now possible to understand the general structure of the calculation with arbitrary value of the angular momentum m. One has the general algebraic equation

$$C' - E' + A'\rho^2 + \frac{B' + m^2 - \frac{1}{4}}{\rho^2} = 2a\left(2m + 2b + 1\right) + 4a^2\rho^2 + \frac{\left(b+m\right)\left(b+m-1\right)}{\rho^2}, \tag{25}$$

which yields the equations:

$$B' + m^2 - \frac{1}{4} = \left(b+m\right)\left(b+m-1\right),\ A' = 4a^2,\ -E' + C' = 2a(2m+2b+1). \tag{26}$$

Finally, the general formula for energy eigenvalue reads

$$E_m = C + \sqrt{\frac{2\hbar^2 A}{\mu}}\left(1 + \sqrt{\frac{2\mu B}{\hbar^2} + m^2}\right),\ m = 0, 1, 2, \cdots \tag{27}$$

and the corresponding normalized radial wave function is factorized in the form

$$\psi_m(\rho,\varphi) = N \exp\left[-\frac{1}{2}\sqrt{\frac{2\mu A}{\hbar^2}}r^2\right] r^{\sqrt{\frac{2\mu B}{\hbar^2}+m^2}} e^{\pm im\varphi},\ m = 0,1,2,\cdots \tag{28}$$

where all normalization constants can be evaluated from the condition

$$\int_0^\infty \left|\psi^{(n)}(r)\right|^2 r dr = 1. \tag{29}$$

For example, the explicit calculation shows that

$$N = \left[\frac{\left(2\sqrt{\frac{2\mu A}{\hbar^2}}\right)^{1+\sqrt{\frac{2\mu B}{\hbar^2}+m^2}}}{\left(\sqrt{\frac{2\mu B}{\hbar^2}+m^2}\right)!}\right]^{1/2}, \tag{30}$$

which is the normalization constant.

2.2 The Mie-type potentials

This potential has been studied in the D dimensions using the polynomial solution and the ansatz wave function method [6,21]. An example on this type of potentials is the standard Morse [30] or Kratzer-Fues [31,32] potential of the form [6,21,24,33]

$$V(\rho) = -D_e\left(\frac{2\rho_e}{\rho} - \frac{\rho_e^2}{\rho^2}\right), \tag{31}$$

where D_e is the dissociation energy between two atoms in a solid and ρ_e is the equilibrium internuclear seperation. The standard Kratzer potential is modified by adding a D_e term to the potential. A new type of this potential is the modified Kratzer-type of molecular potential [21,24]

$$V(\rho) = D_e\left(\frac{\rho-\rho_e}{\rho}\right)^2, \tag{32}$$

and hence it is shifted in amount of D_e. The potential in Eq. (32) has been studied in D dimensions [21] by making the wave function ansatz [20]. However,

this potential has also been discussed before in three dimensions [24] and in D dimensions [6]. This potential [33] can be simply taken as

$$V(r) = \frac{A}{\rho} + \frac{B}{\rho^2} + C, \tag{33}$$

where $A = -D_e r_e$, $B = D_e r_e^2$ and $C = D_e$ [21,24].

First of all, for the ground state ($m = 0$), we take $f_0(\rho) = 1$ and $g(\rho)$ in Eq. (7) to solve Eq. (9)

$$C' - E' + \frac{A'}{\rho} + \frac{B' + m^2 - \frac{1}{4}}{\rho^2} = a^2 + \frac{2ab}{\rho} + \frac{b\,(b-1)}{\rho^2}, \tag{34}$$

where $E' = \frac{2\mu}{\hbar^2}E$, $A' = \frac{2\mu}{\hbar^2}A$, $B' = \frac{2\mu}{\hbar^2}B$ and $C' = \frac{2\mu}{\hbar^2}C$. On equating coefficients of ρ^p, for all $p = -2, 0, 2$, the relations between the potential parameters and the coefficients a and b are

$$B' - \frac{1}{4} = b(b-1),\ A' = 2ab,\ -E' + C' = a^2. \tag{35}$$

Hence, we find from the first equation in (35) that $b = \frac{1}{2} + \sqrt{B'}$ and from the second equation in (35) is solved by $a = \frac{A'}{1+2\sqrt{B'}}$. Finally, the energy eigenvalue reads

$$E_0 = C - \frac{2\mu A^2/\hbar^2}{\left[1 + 2\sqrt{\frac{2\mu B}{\hbar^2}}\right]^2}, \tag{36}$$

and the normalized wave function is

$$\psi_0(\rho, \varphi) = N_0 \exp\left[-\sqrt{-\frac{2\mu}{\hbar^2}\,(E - C)}\rho\right] \rho^{\sqrt{\frac{2\mu B}{\hbar^2}}}. \tag{37}$$

Secondly, for the first node $(m = 1)$, we use $f_1(\rho) = \rho - \alpha_1^{(1)}$ and $g(\rho)$ given in Eq. (7) to solve Eq. (9),

$$C' - E' + \frac{A'}{\rho} + \frac{B' + \frac{3}{4}}{\rho^2} = a^2 + \frac{2a(1+b)}{\rho} + \frac{b\,(b+1)}{\rho^2}. \tag{38}$$

Hence, the relations between the potential parameters and the coefficients a, b and $\alpha_1^{(1)}$ are

$$B' + \frac{3}{4} = b^2 + b,\ A' = 2a(1+b),\ -E' + C' = a^2,\ \alpha_1^{(1)} = 0, \tag{39}$$

and so the exact energy eigenvalue is

$$E_1 = C - \frac{2\mu A^2/\hbar^2}{\left[1 + 2\sqrt{\frac{2\mu B}{\hbar^2} + 1}\right]^2}, \tag{40}$$

and the corresponding wave function is

$$\psi_1(\rho, \varphi) = N_1 \exp\left[-\sqrt{-\frac{2\mu}{\hbar^2}(E - C)}\rho\right] \rho^{\sqrt{\frac{2\mu B}{\hbar^2}+1}} e^{\pm i\varphi}. \tag{41}$$

We follow the same steps for the second node, $m = 2$ (i.e. $f_2(\rho) = (\rho - \alpha_1^{(2)})(\rho - \alpha_2^{(2)})$) and $g(\rho)$ is defined in Eq.(7) to find

$$C' - E' + \frac{A'}{\rho} + \frac{B' + \frac{15}{4}}{\rho^2} = a^2 + \frac{2a(b+2)}{\rho} + \frac{(b+1)(b+2)}{\rho^2}, \tag{42}$$

and their solutions are hence found to be

$$B' + \frac{15}{4} = (b+1)(b+2),\ A' = 2a(b+2),\ -E' + C' = a^2,\ \alpha_1^{(2)} = \alpha_2^{(2)} = 0. \tag{43}$$

Therefore, the energy eigenvalue is

$$E_2 = C - \frac{2\mu A^2/\hbar^2}{\left[1 + 2\sqrt{\frac{2\mu B}{\hbar^2} + 4}\right]^2}, \tag{44}$$

and hence the corresponding wave function is

$$\psi_2(\rho, \varphi) = N_2 \exp\left[-\sqrt{-\frac{2\mu}{\hbar^2}(E - C)}\rho\right] \rho^{\sqrt{\frac{2\mu B}{\hbar^2}+4}} e^{\pm i2\varphi}. \tag{45}$$

Thus, in general, for any arbitrary m, we find that

$$C' - E' + \frac{A'}{\rho} + \frac{B' + m^2 - \frac{1}{4}}{\rho^2} = a^2 + \frac{2a(b+m)}{\rho} + \frac{(b+m)(b+m-1)}{\rho^2}, \tag{46}$$

which leads to the following algebraic equations

$$B' + m^2 - \frac{1}{4} = (b+m)\,(b+m-1)\,,\ A' = 2a(b+m),\ -E' + C' = a^2. \quad (47)$$

Finally, the energy eigenvalue is

$$E_m = C - \frac{2\mu A^2/\hbar^2}{\left[1 + 2\sqrt{\frac{2\mu B}{\hbar^2} + m^2}\right]^2}, \quad (48)$$

and the corresponding normalized wave function is

$$\psi_m(\rho,\varphi) = N \exp\left[-\sqrt{-\frac{2\mu}{\hbar^2}\,(E-C)}\rho\right] \rho^{\sqrt{\frac{2\mu B}{\hbar^2}+m^2}} e^{\pm im\varphi}, \quad (49)$$

where the normalization constant

$$N = \frac{\left(2\sqrt{-\frac{2\mu}{\hbar^2}(E-C)}\right)^{1+\sqrt{\frac{2\mu B}{\hbar^2}+m^2}}}{\sqrt{\left(2\sqrt{\frac{2\mu B}{\hbar^2}+m^2}+1\right)!}}. \quad (50)$$

3 Concluding Remarks

We have easily obtained the exact bound state solutions of the two-dimensional radial Schrödinger equation for two general potential forms representing the pseudoharmonic [5,21] and modified Kratzer molecular [6,21] potentials by using the wave function ansatz method [22,23]. The presented procedure in this study is systematical and efficient in finding the exact energy spectra and corresponding wave functions of the Schrödinger equation for any desired quantum system. This method is simple in producing the exact bound state solution for further anharmonic potentials.

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